Microcanonical Approach to the Simulation of First-Order Phase Transitions.

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A generalization of the microcanonical ensemble suggests a simple strategy for the simulation of first order phase transitions. At variance with flat-histogram methods, there is no iterative parameters optimization, nor long waits for tunneling between the ordered and the disordered phases. We test the method in the standard benchmark: the Q-states Potts model ($Q=10$ in 2 dimensions and $Q=4$ in 3 dimensions), where we develop a cluster algorithm. We obtain accurate results for systems with 10^6 spins, outperforming flat-histogram methods that handle up to 10^4 spins.

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Phase transitions are ubiquitous (formation of quark-gluon plasmas, evaporation/crystallization of ordinary liquids, Cosmic Inflation, etc.). Most of them are of (Ehrenfest) first order [1]. Monte Carlo simulations [2] are crucial for their investigation, but difficulties arise for large system linear size, L (or space dimension, D). The intrinsic problem is that, at a first order phase transition, two (or more) phase coexist. The simulated system tunnels between pure phases by building an interface of size L. The free-energy cost of such a mixed configuration is ΣL^{D-1} (Σ: surface tension), the interface is built with probability $\exp[-\Sigma L^{D-1}]$ and the natural time scale for the simulation grows with L as $\exp[\Sigma L^{D-1}]$. This disaster is called *exponential* critical slowing down (ECSD).

No cure is known for ECSD in canonical simulations (cluster methods [3, 4] do not help), which motivated the invention of the multicanonical ensemble [5]. The multicanonical probability for the energy density is constant, at least in the energy gap $e^{\rm o} < e < e^{\rm d}$ ($e^{\rm o}$ and $e^{\rm d}$: energy densities of the coexisting low-temperature ordered phase and high-temperature disordered phase), hence the name flat-histogram methods [5, 6, 7, 8]. The canonical probability minimum in the energy gap ($\propto \exp[-\Sigma L^{D-1}]$) is filled by means of an iterative parameter optimization.

In flat-histogram methods the system performs an energy random walk in the energy gap. The elementary step being of order L^{-D} (a single spin-flip), one naively expects a tunneling time from $e^{\rm o}$ to $e^{\rm d}$ of order L^{2D} spin-flips. But the (one-dimensional) energy random walk is not Markovian, and these methods suffer ECSD [10]. In fact, for the standard benchmark (the $Q=10$ Potts model [9] in $D=2$), the barrier of 10^4 spins was reached in 1992 [5], while the largest simulated system (to our knowledge) had 4×10^4 spins [6].

ECSD in flat histogram simulations is probably understood [10]: on its way from $e^{\rm d}$ to $e^{\rm o}$, the system undergoes several (four in $D=2$) "transitions". First comes the condensation transition [10, 11], at a distance of order $L^{-D/(D+1)}$ from $e^{\rm d}$, where a macroscopic droplet of the ordered phase is nucleated. Decreasing e, the droplet grows to the point that, for periodic boundary conditions, it reduces its surface energy by becoming a strip [12], see Fig. 2 (in $D=3$, the droplet becomes a cylinder, then a slab [13]). At lower e the strip becomes a droplet of *disordered* phase. Finally, at the condensation transition close to $e^{\rm o}$, we encounter the homogeneous ordered phase.

Here we present a method to simulate first order transitions without iterative parameter optimization nor energy random walk. We extend the configuration space as in Hybrid Monte Carlo [14]: to our N variables, σ_i (named spins here, but they could be atomic positions) we add N real momenta, p_i. The *microcanonical* ensemble for the $\{\sigma_i, p_i\}$ offers two advantages. First, microcanonical simulations [15] are feasible at any value of e within the gap. Second, we obtain Fluctuation-Dissipation Eqs. (5–8) where the (inverse) temperature $\hat\beta$, a function of e and the spins, plays a role dual to that of e in the canonical ensemble. The e dependence of the mean value $\langle\hat\beta\rangle_e$, interpolated from a grid as it is almost constant over the gap, characterizes the transition. We test the method in the Q-states Potts model, for which we develop a cluster algorithm. We handle systems with 10^6 spins for $Q=10$ in $D=2$ and for $Q=4$ in $D=3$ (where multibondic simulations handle $N=10^4$ [17]).

Let U be the spin Hamiltonian. Our total energy is

$$\mathcal{E} = \sum_{i=1}^{N} \frac{p_i^2}{2} \; + \; U \,, \quad (e \equiv \mathcal{E}/N \,,\; u \equiv U/N) \,. \qquad (1)$$

In the canonical ensemble , the $\{p_i\}$ are a trivial gaussian bath decoupled from the spins. Note that, at inverse temperature β, one has $\langle e\rangle_\beta = \langle u\rangle_\beta + 1/(2\beta)$.

Microcanonically, the entropy density, $s(e,N)$, is given by ($\sum_{\{\sigma_i\}}$: summation over spin configurations)

$$\exp[Ns(e,N)] = \int_{-\infty}^{\infty} \prod_{i=1}^{N} {\rm d}p_i \sum_{\{\sigma_i\}} \delta(Ne - \mathcal{E}) \,, \qquad (2)$$

or, integrating out the $\{p_i\}$ using Dirac's delta function,

$$\exp[Ns(e,N)] = \frac{(2\pi N)^{N/2}}{N\Gamma(N/2)} \sum_{\{\sigma_i\}} (e-u)^{\frac{N}{2}-1}\theta(e-u) \,. \qquad (3)$$

The Heaviside step function, $\theta(e-u)$, enforces $e > u$. The microcanonical average at fixed e of a generic function of e and the spins, $O(e,\{\sigma_i\})$, is (see Eq. (3) and [15])

$$\langle O\rangle_e \equiv \frac{\sum_{\{\sigma_i\}} O(e,\{\sigma_i\})\,(e-u)^{\frac{N}{2}-1}\theta(e-u)}{\sum_{\{\sigma_i\}}(e-u)^{\frac{N}{2}-1}\theta(e-u)}\,. \qquad (4)$$

The Metropolis simulation of Eq. (4), is straightforward.

Calculating $\mathrm{d}s/\mathrm{d}e$ from Eq.(3) we learn that [31]

$$\frac{\mathrm{d}s(e,N)}{\mathrm{d}e} \;=\; \langle\hat{\beta}(e;\{\sigma_i\})\rangle_e\,, \qquad (5)$$

$$\hat{\beta}(e;\{\sigma_i\}) \;=\; \frac{N-2}{2N(e-u)}\,. \qquad (6)$$

Fluctuation-Dissipation follows by derivating Eq. (4):

$$\frac{\mathrm{d}\langle O\rangle_e}{\mathrm{d}e} = \left\langle\frac{\partial O}{\partial e}\right\rangle_e + N\left[\langle O\hat{\beta}\rangle_e - \langle O\rangle_e\langle\hat{\beta}\rangle_e\right]\,. \qquad (7)$$

As in the canonical case [18], an integral version of (7) allows to extrapolate $\langle O\rangle_{e'}$ from simulations at $e \geq e'$:

$$\langle O\rangle_{e'} = \frac{\left\langle O(e';\{\sigma_i\})\,\theta(e'-u)\left[\frac{e'-u}{e-u}\right]^{\frac{N}{2}-1}\right\rangle_e}{\left\langle\theta(e'-u)\left[\frac{e'-u}{e-u}\right]^{\frac{N}{2}-1}\right\rangle_e}\,. \qquad (8)$$

For $e < e'$, configurations with $e < u < e'$, suppressed by a factor $(e'-u)^{N/2-1}$, are ignored in (8). Since we are limited in practice to $|e-e'| \leq \sqrt{\langle u^2\rangle_e - \langle u\rangle_e^2}/|\mathrm{d}\langle u\rangle_e/\mathrm{d}e| \sim N^{-1/2}$, the restriction $e \geq e'$ can be dropped, as it is numerically negligible.

The canonical probability density for e, $P_\beta^{(L)}(e) \propto \exp[N(s(e,N)-\beta e)]$ follows from $\langle\hat{\beta}\rangle_e$:

$$\log P_\beta^{(L)}(e_2) - \log P_\beta^{(L)}(e_1) = N\int_{e_1}^{e_2}\mathrm{d}e\,\left(\langle\hat{\beta}\rangle_e - \beta\right)\,. \qquad (9)$$

In the *thermodynamically stable region* (i.e. $\mathrm{d}\langle\hat{\beta}\rangle_e/\mathrm{d}e < 0$), there is a single root of $\langle\hat{\beta}\rangle_e = \beta$, at the maximum of $P_\beta^{(L)}$. But, see Fig. 1, in the energy gap $\langle\hat{\beta}\rangle_e$ has a maximum and a minimum (L-dependent spinodals [1]), and there are several roots of $\langle\hat{\beta}\rangle_e = \beta$. The rightmost (leftmost) root is $e_L^{\mathrm{d}}(\beta)$ ($e_L^{\mathrm{o}}(\beta)$), a local maximum of $P_\beta^{(L)}$ corresponding to the disordered (ordered) phase. We define $e_L^*(\beta)$ as the *second rightmost* root of $\langle\hat{\beta}\rangle_e = \beta$.

At the finite-system (inverse) critical temperature, β_{c}^L, one has [19] $P_{\beta_{\mathrm{c}}^L}^{(L)}(e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L)) = P_{\beta_{\mathrm{c}}^L}^{(L)}(e_L^{\mathrm{o}}(\beta_{\mathrm{c}}^L))$, which is equivalent, Eq. (9) and [20], to Maxwell's construction:

$$0 = \int_{e_L^{\mathrm{o}}(\beta_{\mathrm{c}}^L)}^{e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L)}\mathrm{d}e\,\left(\langle\hat{\beta}\rangle_e - \beta_{\mathrm{c}}^L\right)\,, \qquad (10)$$

(for large N, $\beta_{\mathrm{c}}^\infty - \beta_{\mathrm{c}}^L \propto 1/N$ [21]). Actually, at fixed e in the gap, also $\langle\hat{\beta}\rangle_e$ tends to $\beta_{\mathrm{c}}^\infty$ for large N. In the strip phase it converges faster than β_{c}^L, see Table I.

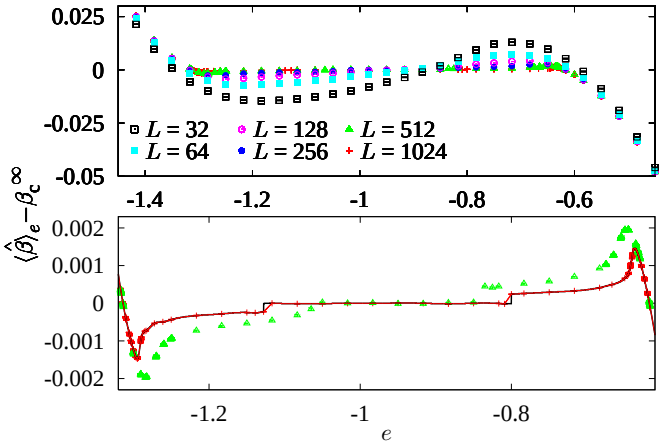

FIG. 1: (Color online) Excess of $\langle\hat{\beta}\rangle_e$ over $\beta_{\mathrm{c}}^{L=\infty}$ vs. e, for the $Q=10$, $D=2$ Potts model and several system sizes. **Bottom:** magnification for $L \geq 512$. The flat central region is the strip phase (the strip width varies at fixed surface free-energy). Lines (shown for $L = 1024$) are the two interpolations used for $L \geq 512$. We connect 3 independent cubic splines, in the strip phase and in its sides, either by a linear function or by a step-like $1/100$ power. Differences among the two interpolations are used to estimate the error induced by the uncertainty in the location of the strip-droplet transitions.

In a cubic box the surface tension is estimated as [32]

$$\Sigma^L = \frac{N}{2L^{D-1}}\int_{e_L^*(\beta_{\mathrm{c}}^L)}^{e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L)}\mathrm{d}e\,\left(\langle\hat{\beta}\rangle_e - \beta_{\mathrm{c}}^L\right)\,. \qquad (11)$$

$L\to\infty$ extrapolations $\Sigma^\infty - \Sigma^L \propto 1/L$ [22] are popular.

As for the specific heat, for $N\to\infty$ the inverse function of the canonical $\langle e\rangle_\beta$ is the microcanonical $\langle\hat{\beta}\rangle_e$:

$$\frac{\mathrm{d}\langle u\rangle_\beta}{\mathrm{d}\beta} \approx \left[\frac{1}{2\langle\hat{\beta}\rangle_e^2} + \frac{1}{\mathrm{d}\langle\hat{\beta}\rangle_e/\mathrm{d}e}\right]_{e=\langle e\rangle_\beta} \equiv C_L(e)\,. \qquad (12)$$

For large N, $e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L)$, $e_L^{\mathrm{o}}(\beta_{\mathrm{c}}^L)$, $C_L(e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L))$, $C_L(e_L^{\mathrm{d}}(\beta_{\mathrm{c}}^L))$ tend to e^{d}, e^{o}, or the specific heat of the coexisting phases (we lack analytical hints about convergence rates).

We now specialize to the Potts model [9]. The spins $\sigma_i = 0, 1, \ldots, Q-1$, live in the $N = L^D$ nodes of a (hyper)cubic lattice of side L with periodic boundary conditions, and interaction ($< ij >$: lattice nearest-neighbors)

$$U = -\sum_{<ij>}\delta_{\sigma_i,\sigma_j}\,. \qquad (13)$$

A cluster method is feasible. Let κ be a tunable parameter and $w(e,u,\kappa) = (e-u)^{N/2-1}\exp[\kappa N u]\theta(e-u)$. Our weight is $w(e,u,\kappa)\exp[-\kappa U]$, see (4), or, introducing bond occupation variables, $n_{ij} = 0, 1$, and $p \equiv 1-\exp[\kappa]$,

$$w(e,u,\kappa)\prod_{<i,j>}\left[(1-p)\delta_{n_{ij},0} \;+\; p\,\delta_{n_{ij},1}\delta_{\sigma_i,\sigma_j}\right]\,, \qquad (14)$$

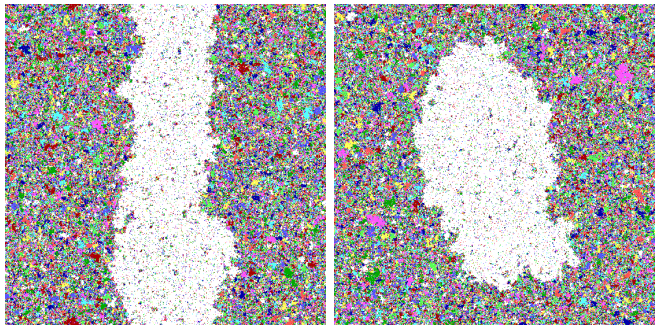

FIG. 2: (Color online) $L = 1024$ equilibrium configurations for the ferromagnetic $Q = 10\,, D = 2$ Potts model with periodic boundary conditions, at the 2 sides of the droplet-strip transition, namely $e = -0.809$ (**left**) and $e = -0.8$ (**right**).

which is the canonical statistical weight at $\beta = \kappa$ [24], but for the $\{n_{ij}\}$ independent factor $w(e, u, \kappa)$. Hence, clusters are traced in the standard way, but we accept a single-cluster flip [4] with Metropolis probability $p(e, \kappa) = \min\{1, w(e, u^{\rm final}, \kappa)/w(e, u^{\rm initial}, \kappa)\}$. Eqs.(5–8) suggest that $\kappa = \langle\hat{\beta}\rangle_e$ maximizes $p(e, \kappa)$ (a short Metropolis run provides a first κ estimate). We obtain $\langle p(e, \kappa)\rangle_e > 0.99$ for $e \le e^{\rm d}$, and still $\langle p(e, \kappa)\rangle_{e=e^{\rm o}} > 0.78$.

We simulated the ($Q = 10$,$D = 2$) Potts model [23], for $L = 32, 64, 128, 256, 512$ and 1024, sampling $\langle\hat{\beta}\rangle_e$ at 30 points evenly distributed in $-1.41666 \le e \le -0.45$. For $L = 512$, we made 15 extra simulations to resolve the narrow spinodal peaks (26 extra points for $L = 1024$). Our Elementary Monte Carlo Step (EMCS) was: $\max\{10, N/(\langle\mathcal{N}\rangle_e\langle p(e, \kappa)\rangle_e)\}$ cluster-flip attempts ($\mathcal{N}$: number of spins in the traced cluster; it is of order one at $e^{\rm d}$ and of order N at $e^{\rm o}$). So, every EMCS we flip at least N spins. For each e, we performed 2×10^6 EMCS, dropping the first 10% for thermalization. A similar computation was carried out for the ($Q = 4$,$D = 3$) Potts model [16] (for details see Table I and [25]).

Our $\langle\hat{\beta}\rangle_e$ in $D = 2$ is shown in Fig. 1. Data reweigthing (8) was used only to reconstruct the narrow spinodal peaks. To find the roots of $\langle\hat{\beta}\rangle_e = \beta$, or to calculate the integrals in Eqs. (10,11), we interpolated $\langle\hat{\beta}\rangle_e$ using a cubic spline [33]. For $L \ge 512$ the strip-droplet transitions produce two "jumps" in $\langle\hat{\beta}\rangle_e$, causing oscillations in the interpolation (Gibbs phenomenon), cured by either of two interpolation schemes, see Fig. 1.

We obtain $\beta_{\rm c}^L$, Σ^L, $e_L^{\rm o}(\beta_{\rm c}^L)$, $e_L^{\rm d}(\beta_{\rm c}^L)$, $C_L(e_L^{\rm o}(\beta_{\rm c}^L))$ and $C_L(e_L^{\rm d}(\beta_{\rm c}^L))$ from the interpolation of $\langle\hat{\beta}\rangle_e$, and of $\mathrm{d}\langle\hat{\beta}\rangle_e/\mathrm{d}e$, see (7). Statistical errors are Jack-Knife's [26] (the i-th block is obtained interpolating the i-th Jack-Knife blocks for $\langle\hat{\beta}\rangle_e$). There are also interpolation and integration errors. Fortunately, errors of order ϵ in $e_L^{\rm o}(\beta_{\rm c}^L)$ or $e_L^{\rm d}(\beta_{\rm c}^L)$ yield errors of order ϵ^2 in $\beta_{\rm c}^L$: the main error in $\beta_{\rm c}^L$ is the quadrature error for $\langle\hat{\beta}\rangle_e$ divided by the latent heat. On the other hand, $e_L^*(\beta_{\rm c}^L)$ is near to the droplet-strip transition, and an error on it does have an impact on Σ_L.

In Table I are our results for ($D = 2, Q = 10$) and the known large L limits. A fit for c in $\beta_{\rm c}^\infty - \beta_{\rm c}^L = c/L^D$ [21] is unacceptable for $L \ge 32$ ($\chi^D/\mathrm{d.o.f.} = 14.32/4$), but good for $L \ge 64$ ($\chi^D/\mathrm{d.o.f.} = 1.77/3$): our accuracy allows to detect subleading corrections. A fit $e_L^{\rm o}(\beta_{\rm c}^L) - e^{\rm o} = b_1/L^D$ works only for $L \ge 256$ ($\chi^2/\mathrm{d.o.f.} = 1.90/2$; for $e_L^{\rm d}(\beta_{\rm c}^L)$ we get $\chi^2/\mathrm{d.o.f.} = 1.41/2$). However, $\beta^{{\rm strip},L}$ (see caption to Table I) is compatible with $\beta_{\rm c}^\infty$ for $L \ge 256$. Then, the simplest strategy to get $\beta_{\rm c}^\infty$ and the latent heat is: (1) for L large enough to display a strip phase, locate it with short runs, (2) get $\beta^{{\rm strip},L}$ accurately, and (3) find the leftmost(rightmost) root for $\langle\hat{\beta}\rangle_e = \beta^{{\rm strip},L}$.

As for Σ^L, the inequality $\Sigma^\infty \le 0.0473505$ [27] (equality under the hypothesis of complete wetting) was violated by $1/L$ extrapolations performed with $L \le 100$ [5]. The reader may check (Table I) that our data for $L \le 256$ extrapolate above 0.0473505, but drop below for $L \ge 512$. Indeed, the consistency of our results for $\beta_{\rm c}^L$ imply that the integration error for $\langle\hat{\beta}\rangle_e$ is (at most) 2×10^{-6} for $L = 1024$. Hence, the integration error for Σ_L is at most 10^{-3}. Adding it to the difference between the linear and the step-like interpolation, Fig. 1, we obtain $\Sigma^{L=1024} = 0.043(2)$, which is slightly below 0.0473505.

As for ($Q = 4$, $D = 3$), see Table I, $\beta^{{\rm strip},L}$ has converged (within accuracy) for $L \ge 64$. Hence, our preferred estimate is $\beta_{\rm c}^\infty = 0.6286206(10)$, that may be compared with Janke and Kapler's $\beta_{\rm c}^\infty = 0.62863(2)$ [16]. Accordingly, we find $e^{\rm o}(\beta^{{\rm strip},L}) = -1.10537(4)$, $e^{\rm d}(\beta^{{\rm strip},L}) = -0.52291(2)$, $C_L(e^{\rm o}(\beta^{{\rm strip},L})) = 35.4(9)$, and $C_L(e^{\rm d}(\beta^{{\rm strip},L})) = 4.24(18)$. The reader will note that $\beta_{\rm c}^{L=128}$ is far too high (for instance, from the χ^2/d.o.f. of the extrapolation $\beta_{\rm c}^L = \beta_{\rm c}^\infty + cL^{-D}$). Therefore, the integration error is $\sim 4 \times 10^{-6}$ (larger than the statistical one), which provides a bound for the error in the surface tension: $\Sigma^{L=128} = 0.0118(4)$. This is compatible with $\Sigma^{L=64}$, and provides a reasonable Σ^∞.

We propose a microcanonical strategy for the Monte Carlo simulation of first-order phase transitions. The method is demonstrated in the standard benchmarks: the $Q = 10$, $D = 2$ Potts model (where we compare with exact results), and the $Q = 4$, $D = 3$ Potts model. For both, we obtain accurate results in systems with more than 10^6 spins (preexisting methods handle 10^4 spins). Envisaged applications include first-order transitions with quenched disorder [16, 28], colloid crystallization [29], peptide aggregation [30] and the condensation transition [11].

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L^D	β_c^L	Σ^L	$-e_L^o(\beta_c^L)$	$-e_L^d(\beta_c^L)$	$-C_L(e_L^o(\beta_c^L)$	$-C_L(e_L^d(\beta_c^L))$	$\beta^{\rm strip,L}$
32^2	1.423082(17)	0.05174(9)	1.3318(2)	0.5736(3),	5.13(13)	3.99(7)	1.42028(7)
64^2	1.425287(9)	0.05024(11)	1.3220(2)	0.5999(2)	6.44(17)	5.78(19)	1.42479(4)
128^2	1.425859(7)	0.049225(14)	1.31676(16)	0.61164(16)	7.4(3)	7.8(3)	1.42592(2)
256^2	1.426021(5)	0.0488(2)	1.31478(8)	0.61578(8)	8.0(3)	8.7(4)	1.42606(2)
$512^{2(A)}$	1.426051(4)	0.0473(3)	1.31392(6)	0.61710(4)	8.6(4)	9.1(4)	1.426048(12)
$512^{2(B)}$	1.426048(4)	0.0467(4)	1.31390(6)	0.61708(5)	8.6(4)	9.1(4)	1.426048(12)
$1024^{2(A)}$	1.4260599(19)	0.0430(3)	1.31375(3)	0.61748(3)	9.7(5)	8.7(4)	1.426066(9)
$1024^{2(B)}$	1.4260600(18)	0.0424(2)	1.31375(3)	0.61748(3)	9.7(5)	8.7(4)	1.426066(9)
∞^2	1.4260624389...	$\Sigma^\infty \le 0.0473505$	1.3136366978...	0.6175872662...	—	—	1.4260624389...
8^3	0.627394(7)	0.005591(10)	1.1553(7)	0.51412(12)	23.0(5)	3.856(16)	0.62625(4)
16^3	0.628440(3)	0.007596(6)	1.1189(4)	0.51818(5)	30.1(8)	3.620(13)	0.626687(15)
32^3	0.6285957(10)	0.009824(6)	1.10751(15)	0.522066(16)	34.2(9)	4.019(17)	0.627889(6)
64^3	0.6286133(7)	0.011557(6)	1.10542(8)	0.522831(8)	33.2(9)	4.11(2)	0.628621(3)
$128^{3(A)}$	0.6286237(5)	0.011778(7)	1.10548(3)	0.52293(2)	35.4(9)	4.25(17)	0.6286206(10)
$128^{3(B)}$	0.6286239(5)	0.011674(9)	1.10549(2)	0.52293(2)	35.4(9)	4.25(17)	0.6286206(10)

TABLE I: System size dependent estimates of the quantities characterizing the first order transition, as obtained for the $Q=10, D=2$ Potts model (**top**) and $Q=4, D=3$ (**bottom**). Errors are Jack-Knife's. Also shown is $\beta^{\rm strip,L}=\langle\hat{\beta}\rangle_{e=-0.95}$ (for $D=2$) or $\beta^{\rm strip,L}=\langle\hat{\beta}\rangle_{e=-0.764443}$ (for $D=3$), in the strip phase. The ∞^2 row contains exact results [23] and an inequality [27], for $D=2$, $Q=10$. The results with superscript $A(B)$ were obtained with the linear(step-like) interpolation scheme, see Fig. 1.

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[31] In [7], Eq. (5) was approximated as $\mathrm{d}s/\mathrm{d}e \approx 1/\langle 1/\hat{\beta}\rangle_e$.

[32] In the strip phase (Fig. 2) *two* interfaces form, hence [22] $P^{(L)}_{\beta_c^L}(e_L^{\rm d}(\beta_c^L))/P^{(L)}_{\beta_c^L}(e_L^*(\beta_c^L)) = \exp[2\Sigma_L L^{D-1}]$.

[33] Not the so called natural spline. We fixed the derivative at the first(last) e value, from a 3 points parabolic fit.